THEOCHEM, VOLUME 40 (1988)

(*Journal of Molecular Structure, Vol. 163*)

AUTHOR INDEX

Arrington, C. A. 191

Balaji, V. 191
Batra, I. P. 63
Bernardi, F. 173
Bertrán, J. 101
Bodor, N. 315
Bofill, J. M. 285
Borden, W. T. 51
Bottoni, A. 173
Bozlee, B. 239

Chattopadhyay, A. 63
Chen, H.-T. E. 89

Denton, J. 355
Dieter, K. 143
Doubleday, Jr., C. 331
Downing, J. W. 191
Duran, M. 389

Endo, J. 249

Fischer, C. R. 63
Fox, M. A. 163
Fujimoto, H. 249
Fukui, K. 249

Galera, S. 101
Glaser, R. 19
Gleicher, G. J. 239
Goddard, III, W. A. 207
Gomez, J. 285
Greenberg, A. 89
Griller, D. 125

Halgren, T. A. 429
Halvick, P. 267
Horowitz, D. S. 207
Hrovat, D. A. 51

Kaminski, J. J. 315
Kanabus-Kaminska, J. M. 125

Lee, C. 305
Liebman, J. F. 89
Lluch, J. M. 101
Lyu, P.-C. 89

Maccoll, A. 125
Madhavan, P. V. 63
Mahiou, B. 239
McCourt, M. 343, 355
McIver, Jr., J. W. 331, 343, 355
Michl, J. 191
Miller, M. A. 133
Minchin, S. A. 239
Mizutani, Y. 249
Murcko, M. A. 1
Murdoch, J. R. 447
Murray, J. S. 111
Murthy, G. S. 191

Nobes, R. H. 151

Oliva, A. 101
Olivella, S. 285
Osamura, Y. 389

Page, M. 331
Parr, R. G. 305
Politzer, P. 111

Radom, L. 151
Radziszewski, J. G. 191
Rayez, J. C. 267
Reynolds, C. H. 79

Schaefer, III, H. F. 389
Schulman, J. M. 133
Smith, K. A. 259
Soppe-Mbang, H. 239
Spurgeon, C. J. 239
Stewart, J. J. P. 143
Stoecklin, T. 267
Streitwieser, Jr., A. 19, 259
Sun, H. 51

Thiel, W. 415

Venturini, A. 173

Whitten, J. L. 63
Wiberg, K. B. 1
Wong, M. W. 151

Yamaguchi, Y. 389
Yang, W. 305
Younathan, J. N. 163

THEOCHEM VOLUME 40 (1988)

(*Journal of Molecular Structure, Vol. 163*)

SUBJECT INDEX

Active region,
a study on the active region of molecules and chemical reactivity 249
Ammonium ion,
an AM1 study of the preferential solvation of ammonium ion in ammonia—water mixtures 101
Asteranes,
AM1, MNDO and MM2 studies of concatenated cyclobutanes: prismanes, ladderanes and asteranes 133

Bicyclo[2,1,0]pent-2-ene,
reinvestigation of some thermally "forbidden" pericyclic reactions and biradical processes in the semiempirical TCSCF approach. Part 1. Disrotatory opening of cyclobutene, isomerization of bicyclo[2,1,0]pent-2-ene and dimerization of ethylene to cyclobutane 285
Bond dissociation energies,
bond dissociation energies for common organic compounds 125

Cartesian derivatives,
new formulas for integrals in semiempirical molecular orbital methods. Part 2. Coulomb integrals and their first and second Cartesian derivatives in the NDDO theory 355
Cartesian nuclear displacements,
new formulas for integrals in semiempirical molecular orbital methods. Part 1. General theory and results for two center overlap integrals and their first and second derivatives with respect to Cartesian nuclear displacements 343
Chemical reactivity,
a study on the active region of molecules and chemical reactivity 249
chemical reactivity predictions from molecular structures and properties. Perturbation approaches to electronic and structural rearrangements 447
CO,
local softness and chemical reactivity in the molecules CO, SCN^- and H_2CO 305
Conjugated cations,
a MNDO study of the geometries and rotational barriers of conjugated cations and radical cations 163
$C(^3P) + SH(X^2\pi)$,
theoretical study of the reaction $C(^3P) + SH(X^2\pi)$. Part 1. Semi-quantitative determination of some parts of the potential energy surfaces 267
Cyclobutanes,
AM1, MNDO and MM2 studies of concatenated cyclobutanes: prismanes, ladderanes and asteranes 133
Cyclobutene,
reinvestigation of some thermally "forbidden" pericyclic reactions and biradical processes in the semiempirical TCSCF approach. Part 1. Disrotatory opening of cyclobutene, isomerization of bicyclo[2,1,0]pent-2-ene and dimerization of ethylene to cyclobutane 285

Dihydropyridines,
correlation between hydride transfer and one-electron oxidation of dihydropyridines and heterocycles 315
Dioxins,
calculated structures and electrostatic potentials of some monocyclic unsaturated dioxins 111
Dynamic reaction coordinates,
calculation of vibrational frequencies using molecular trajectories 143

Ethylene,
reinvestigation of some thermally "forbidden" pericyclic reactions and biradical processes in the semiempirical TCSCF approach. Part 1. Disrotatory opening of cyclobutene, isomerization of bicyclo[2,1,0]pent-2-ene and dimerization of ethylene to cyclobutane 285

Force constants,
maximally diagonal force constants in dependent angle-bending coordinates. Part I. Mathematical formulation 431

2-Haloethanols,
rotational barriers. Part 3. 2-Haloethanols 1
H_2CO,
local softness and chemical reactivity in the molecules CO, SCN^- and H_2CO 305
$[HCS]^+$,
the $[HCS]^+$ and $[H_2CS]^{2+}$ potential energy surfaces: predictions of bridged equilibrium structures 151
$[H_2CS]^{2+}$,
the $[HCS]^+$ and $[H_2CS]^{2+}$ potential energy surfaces: predictions of bridged equilibrium structures 151
Heterocycles,
correlation between hydride transfer and one-electron oxidation of dihydropyridines and heterocycles 315

Inverse sandwich compounds,
inverse sandwich compounds 259
Iodomethylarenes,
the reaction of iodomethylarenes with triphenyltin radical. Use of molecular orbital modelling to evaluate the rate determining step 239

Ladderanes,
AM1, MNDO and MM2 studies of concatenated cyclobutanes: prismanes, ladderanes and asteranes 133

Lithiated oxime ethers,
a MNDO-study of solvent-free and solvated dimeric lithium ion pairs of acetaldoxime. Models for dimeric aggregates of lithiated oxime ethers 19
Lithium ion pairs,
a MNDO-study of solvent-free and solvated dimeric lithium ion pairs of acetaldoxime. Models for dimeric aggregates of lithiated oxime ethers 19

Normal coordinates
Calculation of vibrational frequencies using molecular trajectories 143

Prismanes,
substituent effects of the geometries of prismanes 89
AM1, MNDO and MM2 studies of concatenated cyclobutanes: prismanes, ladderanes and asteranes 133

Radical cations,
a MNDO study of the geometries and rotational barriers of conjugated cations and radical cations 163
Rotational barriers,
rotational barriers. Part 3. 2-Haloethanols 1

Sandwich compounds,
inverse sandwich compounds 259
SCF-MO study,
an ab initio SCF-MO study of the aromaticity of some cyclic compounds 173
SCN^-,
local softness and chemical reactivity in the molecules CO, SCN^- and H_2CO 305
Self-consistent-field wavefunctions,
analytical energy third derivatives for two-configuration self-consistent-field wavefunctions 389
Semiempirical geometry,
fast semiempirical geometry optimizations 415
Si(111),
surface π bonding in the (2×1) reconstruction of Si(111) 63
Silicon-containing molecules,
theoretical studies of silicon-containing molecules 207
Si—Si double bond,
ab initio study of rotation about the Si—Si double bond in disilene 51
Substituted benzenes,
modeling of shape/size selective separations: AM1 rotational barriers for some substituted benzenes 79

Tetramethylene,
dynamics of singlet biradicals. Applications of ab initio variational transition state theory to the fragmentation of tetramethylene 331
Trajectories,
calculation of vibrational frequencies using molecular trajectories 143
Triphenyltin radical,
the reaction of iodomethylarenes with triphenyltin radical. Use of molecular orbital modelling to evaluate the rate determining step 239

Vibrational frequencies,
calculation of vibrational frequencies using molecular trajectories 143

Vibrational transition moment directions,
vibrational transition moment directions in medium-size molecules: experiment and theory 191

CONTENTS

Dedication: Professor M. J. S. Dewar ix

Rotational barriers. Part 3. 2-Haloethanols
K. B. Wiberg and M. A. Murcko (New Haven, CT, U.S.A.) 1

A MNDO-study of solvent-free and solvated dimeric lithium ion pairs of acetaldoxime. Models for dimeric aggregates of lithiated oxime ethers
R. Glaser and A. Streitwieser, Jr. (Berkeley, CA, U.S.A.) 19

Ab initio study of rotation about the Si—Si double bond in disilene
D. A. Hrovat, H. Sun and W. T. Borden (Seattle, WA, U.S.A.) 51

Surface π bonding in the (2 × 1) reconstruction of Si(111)
A. Chattopadhyay, P. V. Madhavan, J. L. Whitten (Stony Brook, NY, U.S.A.), C. R. Fischer (Flushing, NY, U.S.A.) and I. P. Batra (San Jose, CA, U.S.A.) 63

Modeling of shape/size selective separations: AM1 rotational barriers for some substituted benzenes
C. H. Reynolds (Spring House, PA, U.S.A.) 79

Substituent effects of the geometries of prismanes
A. Greenberg, H.-T. E. Chen, P.-C. Lyu (Newark, NJ, U.S.A.) and J. F. Liebman (Baltimore, MD, U.S.A.) . . . 89

An AM1 study of the preferential solvation of ammonium ion in ammonia—water mixtures
S. Galera, J. M. Lluch, A. Oliva and J. Bertrán (Barcelona, Spain) 101

Calculated structures and electrostatic potentials of some monocyclic unsaturated dioxins
J. S. Murray and P. Politzer (New Orleans, LA, U.S.A.) 111

Bond dissociation energies for common organic compounds
D. Griller, J. M. Kanabus-Kaminska (Ottawa, Ontario, Canada) and A. Maccoll (London, Gt. Britain). 125

AM1, MNDO and MM2 studies of concatenated cyclobutanes: prismanes, ladderanes and asteranes
M. A. Miller and J. M. Schulman (Flushing, NY, U.S.A.). 133

Calculation of vibrational frequencies using molecular trajectories
K. Dieter and J. J. P. Stewart (Colarado Springs, CO, U.S.A.). 143

The $[HCS]^+$ and $[H_2CS]^{2+}$ potential energy surfaces: predictions of bridged equilibrium structures
M. W. Wong, R. H. Nobes and L. Radom (Canberra, A.C.T., Australia) 151

A MNDO study of the geometries and rotational barriers of conjugated cations and radical cations
J. N. Younathan and M. A. Fox (Austin, TX, U.S.A.) 163

An ab initio SCF-MO study of the aromaticity of some cyclic compounds
F. Bernardi, A. Bottoni and A. Venturini (Bologna, Italy). 173

Vibrational transition moment directions in medium-size molecules: experiment and theory
J. G. Radziszewski, C. A. Arrington, J. W. Downing, V. Balaji, G. S. Murthy and J. Michl (Austin, TX, U.S.A.) 191

Theoretical studies of silicon-containing molecules
D. S. Horowitz and W. A. Goddard III (Pasadena, CA, U.S.A.) 207

The reaction of iodomethylarenes with triphenyltin radical. Use of molecular orbital modelling to evaluate the rate determining step
G. J. Gleicher, C. J. Spurgeon, B. Mahiou, H. Soppe-Mbang, B. Bozlee and S. A. Minchin (Corvallis, OR, U.S.A.) 239

A study on the active region of molecules and chemical reactivity
H. Fujimoto, J. Endo, Y. Mizutani and K. Fukui (Kyoto, Japan). 249

Inverse sandwich compounds
A. Streitwieser, Jr. and K. A. Smith (Berkeley, CA, U.S.A.). 259

Theoretical study of the reaction $C(^3P) + SH(X^2\pi)$. Part 1. Semi-quantitative determination of some parts of the potential energy surfaces
T. Stoecklin, P. Halvick and J. C. Rayez (Talence, France) 267

(continued overleaf)

(contents continued)

Reinvestigation of some thermally "forbidden" pericyclic reactions and biradical processes in the semiempirical TCSCF approach. Part 1. Disrotatory opening of cyclobutene, isomerization of bicyclo[2,1,0]pent-2-ene and dimerization of ethylene to cyclobutane
J. M. Bofill, J. Gomez and S. Olivella (Barcelona, Spain) 285

Local softness and chemical reactivity in the molecules CO, SCN^- and H_2CO
C. Lee, W. Yang and R. G. Parr (Chapel Hill, NC, U.S.A.) 305

Correlation between hydride transfer and one-electron oxidation of dihydropyridines and heterocycles
N. Bodor (Gainesville, FL, U.S.A.) and J. J. Kaminski (Bloomfield, NJ, U.S.A.) 315

Dynamics of singlet biradicals. Application of ab initio variational transition state theory to the fragmentation of tetramethylene
C. Doubleday, Jr. (New York, NY, U.S.A.), M. Page (Washington, DC, U.S.A.) and J. W. McIver, Jr. (Buffalo, NY, U.S.A.) 331

New formulas for integrals in semiempirical molecular orbital methods. Part 1. General theory and results for two center overlap integrals and their first and second derivatives with respect to Cartesian nuclear displacements
M. McCourt and J. W. McIver, Jr. (Buffalo, NY, U.S.A.) 343

New formulas for integrals in semiempirical molecular orbital methods. Part 2. Coulomb integrals and their first and second Cartesian derivatives in the NDDO theory
J. Denton, M. McCourt and J. W. McIver, Jr. (Buffalo, NY, U.S.A.) 355

Analytical energy third derivatives for two-configuration self-consistent-field wavefunctions
M. Duran, Y. Yamaguchi, Y. Osamura and H. F. Schaefer III (Berkeley, CA, U.S.A.) 389

Fast semiempirical geometry optimizations
W. Thiel (Wuppertal, F.R.G.) 415

Maximally diagonal force constants in dependent angle-bending coordinates. Part I. Mathematical formulation
T. A. Halgren (Rahway, NJ, U.S.A.) 431

Chemical reactivity predictions from molecular structures and properties. Perturbation approaches to electronic and structural rearrangements
J. R. Murdoch (Wilmington, DE, U.S.A.) 447

Author Index 477

Subject Index 479